

Spectral regression and correlation coefficients of some benzaldimines and salicylaldimines in different solvents

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Abstract

Sixteen Schiff bases obtained from the condensation of benzaldehyde or salicylaldehyde with various amines (aniline, 4-carboxyaniline, phenylhydrazine, 2,4-dinitrophenylhydrazine, ethylenediamine, hydrazine, *o*-phenylenediamine and 2,6-pyridinediamine) are studied with UV–vis spectroscopy to observe the effect of solvents, substituents and other structural factors on the spectra. The bands involving different electronic transitions are interpreted. Computerized analysis and multiple regression techniques were applied to calculate the regression and correlation coefficients based on the equation that relates peak position λ_{\max} to the solvent parameters that depend on the H-bonding ability, refractive index and dielectric constant of solvents.

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1. Introduction

The research on Schiff base compounds is growing because of their biological importance [1–3]. Recently, Co(III) complexes with Schiff bases were reported as a new anticancer agents with radio/thermosensitizing activities [4]. It was also found that Co–salen complexes bound to DNA in an intercalative model supported by fluorescence spectral studies (salen is bis(salicylidene)ethylenediamine) [5].

The study of solvent effects on the UV absorption spectra of Schiff bases has received great deal of attention. The benzaldimines studied are: substituted *N*-(*R*-benzylidene)benzidine and *N*-(*R*-furfurylidene)benzidine [6], *N*-benzylidene and *N*-naphthylbenzylidene-2-aminopyrimidine [7] bis(*X*-benzylidene-*o*-phenylenediamine [8]. Salicylaldimines show important photochromism where light absorption causes interconversion between enol-imine and keto-amine tautomers through intramolecular hydrogen transfer. Several spectroscopic studies on the photochromisms of salicylaldimines of different structures were under-

taken: *N,N'*-bis(salicylidene)-1,2-diaminoethane and *N,N'*-bis(salicylidene)-1,6-hexanediamine [9], *N*-salicylidene-1-hexadecylamine [10], *N,N'*-bis(salicylidene)-1,2-cyclohexanediamine [11] and *N*-salicylidene- α -methylbenzylamine [12]. The tautomeric equilibrium of salicylidene Schiff bases is the subject of considerable interest from both theoretical and practical point of view [13–15]. The position of proton transfer equilibrium in solution is affected by interactions with the solvent molecules. The tendency of interconversion to ketoamine has been observed in polar solvents for *N*-(*R*-salicylidene)-benzylamine [16], *N*-(*R*-salicylidene)-methylamines [17,18] and *N,N'*-bis(salicylidene)-2,6-pyridinediamine [19].

Although UV–vis spectral behavior of Schiff bases have been extensively investigated in recent years, only spare information is available about the effect of different solvent parameters on the position of observed absorption peak [17]. In a continuation of our previous studies of computerized correlation data for the solvent effects on the electronic spectra of organic compounds (barbiturate and azo compounds) [20–25], the present work was undertaken. This paper deals with solvent and structural effects on the UV–vis absorption spectra of 16 Schiff bases derived from benzaldehydes or

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Table 1
Numbers and names of Schiff bases

IA	<i>N</i> -Benzylideneaniline	IB	<i>N</i> -Salicylideneaniline
IIA	<i>N</i> -(4-Carboxyphenyl)benzylideneimine	IIB	<i>N</i> -(4-Carboxyphenyl)salicylideneimine
IIIA	Benzaldehydephenylhydrazone	IIIB	Salicylaldehydephenylhydrazone
IVA	2,4-Dinitrobenzaldehydephenylhydrazone	IVB	2,4-Dinitrosalicylaldehydephenylhydrazone
VA	<i>N,N'</i> -bis(Benzylidene)ethylenediamine	VB	<i>N,N'</i> -bis(Salicylidene)ethylenediamine
VIA	<i>N,N'</i> -bis(Benzylidene)hydrazine	VIB	<i>N,N'</i> -bis(Salicylidene)hydrazine
VIIA	<i>N,N'</i> -bis(Benzylidene)- <i>o</i> -phenylenediamine	VIIIB	<i>N,N'</i> -bis(Salicylidene)- <i>o</i> -phenylenediamine
VIIIA	<i>N,N'</i> -bis(Benzylidene)-2,6-pyridinediamine	VIIIB	<i>N,N'</i> -bis(Salicylidene)-2,6-pyridinediamine

salicylaldehydes and various amines (Table 1; Figs. 1–4). Correlation data was computed in order to evaluate the solvent–solute interaction effects on the electronic absorption spectra of Schiff bases. Several absorption peaks in a single

compound was studied independently by regression analysis and high positive correlation coefficients were obtained. The effect of molecular structures of the compounds on their spectral behavior is also discussed.

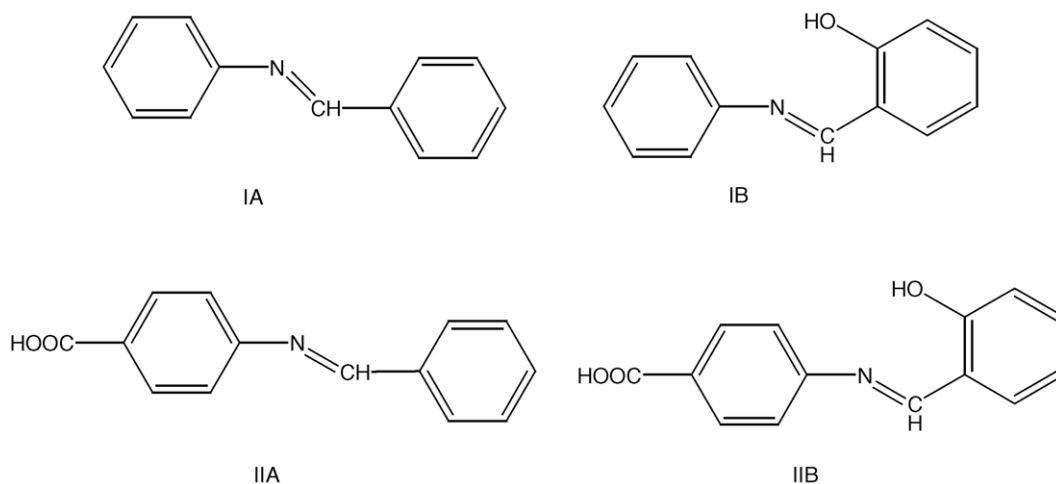


Fig. 1. Structure of Schiff bases IA, IB, IIA and IIB.

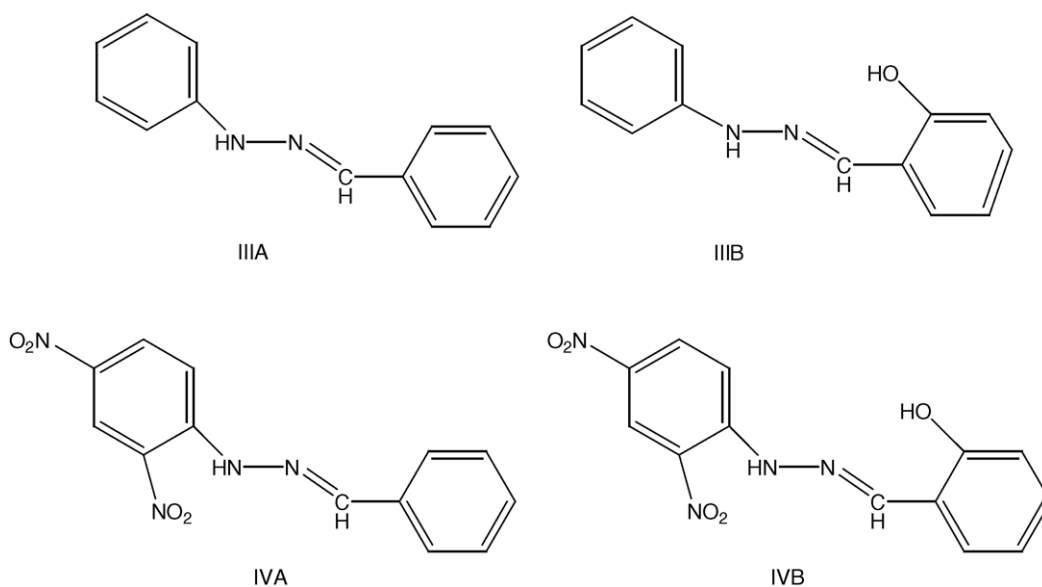


Fig. 2. Structure of Schiff bases IIIA, IIIB, IVA and IVB.

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